



From Iron to Gallium Nitride

# Classical Theory of Crystal Dislocations

Hiroyasu Saka

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B : metalloids  
(1 1 1)  
Groups IV & V

A : metals  
(111)  
Groups II & III

$$A(g) = \langle \beta \rangle (g)$$

$$B(s) = \langle \beta \rangle (s)$$

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$$A(s) = \langle \alpha \rangle (s)$$

$$A(g) = \langle \beta \rangle (g)$$

$$B(s) = \langle \beta \rangle (s)$$

The book consists of two parts: Part 1 is a standard text of dislocation theory. Mathematics is avoided as much as possible. Part 2 describes application of dislocation theory, which includes mechanical properties (including the inverse temperature dependence of strength) and dislocations in functional materials such as Si, GaN and SiC and dislocations in a thin crystal such as an epitaxial layer. This is what has been long anticipated among researchers in industry.

The book contains about 330 illustrations (mostly originals by the author) and the pictures obtained by the author by means of in-situ experiment in a transmission electron microscope over the past 50 years.

This book includes many exercises, which the author found useful when he was teaching in Department of Materials Science and Engineering of Nagoya University to stimulate their interests in dislocation theory.

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$$A(s) = \langle \alpha \rangle (s)$$

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Saka



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**Hiroyasu Saka**

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# **Classical Theory of Crystal Dislocations**

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## Foreword

A crystal consists of atoms or molecules that are arranged regularly in three dimensions. However, in real crystals, this regularity is disturbed, giving rise to disorders. These disorders in crystals are referred to as lattice imperfections (lattice defects). Among the lattice defects, linear defects are referred to as dislocations. Most of the crystals we treat practically contain dislocations. In metallic crystals, dislocations provide plasticity and strength. Dislocations are *friendly* in metallic crystals. In contrast, dislocations in semiconductors are nothing else but *adversary*, deteriorating the optical and electrical properties.

Therefore, the first barrier to overcome in developing semiconductors is to grow crystals as perfect as possible. In the case of silicon, which is by now a commodity in the industry, a vast amount of energy was to be spent before obtaining dislocation-free perfect crystals in its early stage of development. In the case of gallium nitride, which was more recently developed successfully, it is no exaggeration to say that growth of high-quality crystals with a low dislocation density was the key to the success in developing high-performance light-emitting devices and electronic devices.

Science of dislocations, i.e., theory of dislocations, has been well established to explain plasticity of metallic materials. A detailed knowledge on dislocations is essential in the field of semiconductor engineering as well. However, theory of dislocations is quite a difficult science, mastering of which is time-consuming and painstaking. Therefore, those researchers and engineers who are actually being engaged in research and development of novel semiconductor materials have awaited a systematic and yet easy textbook of theory of dislocations.



In view of this, Dr. Hiroyasu Saka published a textbook of dislocation theory that covers fundamentals to cutting-edge applications. The author has studied dislocations by means of transmission electron microscopy over half a century. Thus, in the textbook some of the transmission electron microscopy observations are used, together with generous original diagrams. This is the first textbook that deals with dislocations in cutting-edge semiconductors such as GaAs, SiC, and GaN. In conclusion, it provides the classical theory of dislocation covering from fundamentals to cutting-edge applications in such a style that even beginners can read easily.

I would like to recommend this book as a *bible* to win a battle against dislocations, which will last forever in developing novel materials.

February 2016

Isamu Akasaki *Nagoya Japan*



## Preface

Theory of dislocations is one of the most difficult sciences for students in materials science and engineering (MSE) for the following three reasons:

- (1) Geometrical consideration of dislocation, typical of which is Burgers vector: The definition of Burgers vector appears quite simple, however, it is rather difficult to master its significance completely. Many beginners stumble here.
- (2) Elasticity theory: The concept of dislocations stems from applied mathematics. Thus, it has been taken as granted that advanced mathematics is indispensable to understand the theory of dislocations. This is not necessarily so. It is true that solid state physicists have contributed much towards developing theory of dislocations, but too much mathematics has been required as a prerequisite condition for the beginners to master theory of dislocations. Many, if not all, students in MSE are not good enough in advanced mathematics. This is another reason why students of MSE stay away from theory of dislocations.
- (3) Crystallography: Dislocations are crystal defects. Therefore, it is needless to say that a detailed knowledge of crystallography is indispensable. However, knowledge of traditional crystallography is of little use. It is the crystallography for dislocations, such as Thompson tetrahedron, that is necessary.

Theory of dislocations has contributed much toward understanding plastic behaviour of metallic materials which are important as structural materials. However, there is still a gap between theory and practice not only in a quantitative sense but also in a qualitative sense. For instance, with

regard to controversy on the nature of dislocations in Si, shuffle-glide controversy, the gap is hopelessly wide. Supercomputer is expected to bridge this gap. However, needless to say, in order to make full use of the computer's ability, comprehensive knowledge on classical theory of dislocations is crucial.

On the other hand, a new development is emerging. Importance of dislocations in functional materials is now being recognized. It is well known that reducing the dislocation density in a compound semiconductor GaN was the key to the invention of an LED. Reducing the dislocation density in SiC, a promising candidate for a power device, is also an urgent issue. These materials are quite brittle at room temperature, however, they are surprisingly ductile at high temperatures. In other words, in a high temperature region where these functional materials are processed, behaviour of dislocations is quite spectacular. 'Dislocations are living' literally! It is this understanding that leads to realization of novel functional materials.

In view of these backgrounds, this book is intended:

- (1) to summarize elements of classical theory of crystal dislocations with mathematics kept to a minimum
- (2) to provide a detailed knowledge on behaviour of dislocations in cutting-edge materials, especially semiconductors.

The first seven chapters are devoted to fundamental properties of dislocations in general. Chapters 8–11 are devoted to detailed description of dislocations in different crystal structures of importance. Chapter 12 is devoted to macroscopic strength of materials, in particular, structural materials. A variety of strengthening mechanisms are presented. Chapter 13 is devoted to behaviour of dislocations in thin crystals such as epilayers and transmission electron microscopy (TEM) foil specimens.

The expected audience is twofold. One is students of MSE. The other is researchers and/or engineers who are struggling in reducing the dislocation density in the products they are developing and/or manufacturing. Fortunately, the author has studied dislocations using TEM, some of which are used in this book. He would like to express his hearty thanks to his graduate students and colleagues who took these TEM pictures. Finally, he owes much to Dr. Takashi Saka for discussions in Chapters 3 and 4 and also Dr. Ichiro Yonenaga for discussion on polarity in Chapter 11.

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